

CHAPTER 4

MODEL DOCUMENTATION

The following is a list of modeling groups along with a brief description of the respective models.

Section 4.1	AER 2-D Model	109
Section 4.2	CALJPL 2-D Model	112
Section 4.3	CAMBRAL 2-D Model	113
Section 4.4	CAO 2-D Model	115
Section 4.5	CLKSON 2-D Model	116
Section 4.6	DUPONT 2-D Model	119
Section 4.7	GISS 1-D and 3-D Models	123
Section 4.8	GSFC1 2-D Model	125
Section 4.9	GSFC2- 2-D Model	127
Section 4.10	LARC 3-D Model	130
Section 4.11	LLNL 2-D Model	131
Section 4.12	MPIC 2-D Model	132
Section 4.13	MRI 2-D Model	133
Section 4.14	NOCAR 2-D Model	135
Section 4.15	OSLO 2-D Model	137
Section 4.16	WISCAR 2-D Model	138

Section 4.1 AER 2-D Model

M.K.W. Ko, D. Weisenstein, N.D. Sze
Atmospheric and Environmental Research, Inc.
840 Memorial Drive
Cambridge, Massachusetts 02139
(617) 547-6207

Description of the AER 2-D Photochemical Transport Model

Model Domain and Resolution

The AER 2-D model domain extends from south pole to north pole and approximately from the ground to 55 km. Latitude (ϕ) and the logarithm of the equilibrium pressure ($\zeta = \log(p_o/p_e)$, $p_o = 1000$ mb) are used as coordinates. The equilibrium pressure, p_e , is a pressure-like variable which is a function of potential temperature (θ) defined as

$$p_e = p_o \left[\frac{T_e}{\theta} \right]^{\frac{1}{k}}$$

where T_e is latitudinally-averaged radiative equilibrium temperature, $k = R/c_p$. The model grid uses 19 latitudes and 17 heights. The latitudinal resolution is approximately 9.5 degrees. The vertical levels are constant in ζ with $\Delta\zeta = 0.5$, corresponding to approximately 3 km. The coordinates for the grid point (i,j) at the center of the box are defined in latitude and equilibrium pressure as follows:

$$\phi = \left[(i - 10) * \frac{180}{19} \right], \quad i = 1, 19$$

$$p_e = 1000 * \exp(-.5 * j + .25), \quad j = 1, 17$$

The grid boxes are centered one-half space away from model boundaries. Tracer concentrations are defined at grid box centers and fluxes are defined at grid box edges.

Transport Treatment

Dynamical transport within the model is affected by the zonal-mean diabatic circulation, by quasi-horizontal diffusion along isentropic surfaces, and by vertical diffusion in the troposphere and upper stratosphere. The diabatic circulation was derived by combining the calculated heating rates from Murgatroyd and Singleton (1961) for the upper stratosphere and Dopplack (1979) for the lower stratosphere into a sum of hyperbolic secant functions which is continuous over the model domain. Tracer concentrations depend critically on the details of the circulation in the lower stratosphere, where heating rates are small (less than 1°/day) and poorly determined. Our diabatic heating rates resemble those derived by Rosenfeld et al. (1987) in both structure and magnitude. The vertical velocity is derived from the diabatic heating by:

$$w_e = -\rho g \frac{Q}{\Gamma}$$

where $w_e = dp_e/dt$, ρ is the air density, g the gravitational acceleration, Q the diabatic heating rate, and Γ the static stability parameter. To ensure mass continuity, w_e has to be adjusted so that the global average of w_e along a p_e surface vanishes. This is approximately equivalent to adjustment of Q to ensure that the global average heating vanishes. Horizontal motions are derived from continuity:

$$\frac{1}{a \cos \phi} \frac{\partial}{\partial \phi} (v \cos \phi) + \frac{\partial w_e}{\partial p_e} = 0$$

where a is the earth's radius. The stream function, defined by:

$$\psi(p_e, \phi) = \int_{-90}^{\phi} w_e(p_e, \phi') a \cos \phi' d\phi'$$

is determined for four seasons and interpolated every time step.

The horizontal eddy diffusion coefficient, K_{yy} , for the troposphere and lower stratosphere varies from 3×10^9 cm²/sec at low latitudes to 6×10^9 cm²/sec at mid-latitudes in fall and winter or 2×10^{10} cm²/sec at mid-latitudes in spring and summer. These values yield a good fit to observed ozone profiles in the lower stratosphere and are close to the magnitudes derived by Newman and Schoeberl (1986). The value of K_{yy} in the stratosphere above 25 km is 3×10^9 cm²/sec for all latitudes and seasons. This is based on the work of Kida (1983) and Tung (1984) in estimating an average horizontal diffusion coefficient for the stratosphere.

The vertical diffusion coefficient is 1×10^5 cm²/sec in the troposphere, 1×10^3 cm²/sec in the stratosphere below 40 km, and 1×10^4 cm²/sec above 40 km. The relatively large vertical diffusion coefficient in the troposphere simulates convective overturning and synoptic scale eddies. Stratospheric vertical diffusion was estimated by Kida (1983) to be 1×10^3 cm²/sec. Enhanced vertical mixing above 40 km is based on the work of Garcia and Solomon (1985) regarding gravity wave breaking.

Chemical Treatment

The chemistry scheme contains about 50 chemical species which interact through 130 reactions. Reactions for the oxygen, hydrogen, methyl, nitrogen, and chlorine families are included in all model calculations. Chemistry for bromine and fluorine species can be included as an option. Water vapor concentration is not calculated, but is parameterized in the stratosphere based on the Nimbus 7 observations of Remsberg et al. (1984). The tropospheric values of H₂O vary seasonally depending on the parameterized value of relative humidity.

The chemical scheme employs the grouping technique to deal with chemicals having vastly different atmospheric lifetimes. Short-lived species are always in chemical equilibrium with their surroundings and their concentrations vary diurnally. Long-lived species vary only on the scale of weeks or months and therefore are affected by atmospheric motions.

The AER 2-D model does explicit diurnal calculations of the short-lived chemical species. An iterative newton scheme is used to solve for all the fast species simultaneously, making 10 steps for the daylight hours and 5 steps for the nighttime hours until 24-hour periodicity is reached. The fast species are computed for a given day while holding the sum of the odd chlorine species, the sum of the odd nitrogen species, and the concentrations of other slow species fixed. Production and loss rates for the slow species are then computed. These production and loss rates are used to compute the chemical source terms (production rate and loss frequency) in the advection equation for the next 10 days of model simulation.

The kinetic reaction rates and absorption cross sections are those given by NASA/JPL (1987). The solar fluxes are from WMO/NASA (1982). The spectral resolution is 5 nm or less over the wavelength range from 93 nm to 405 nm. Photolysis rates were computed with allowance for the effects of Rayleigh

Section 4.2 CALJPL 2-D Model

Y.L. Yung, D. Crisp, and R.W. Zurek
California Institute of Technology and Jet
Propulsion Laboratory

Model Domain and Resolution

Height: 0-80 km (variable), -2 km resolution, log p coordinate

Latitude: Pole-to-Pole, $\Delta\theta = 10^\circ$ (variable)

Transport Treatment: Modular Radiative-Dynamic-Chemical Model

Residual-mean stream function algorithm

Net Heating computed by independent radiation code

Mass continuity equation solved using Prather's method

Chemistry taken from 1-D Caltech model (45 species)

Radiation:

Complete "physical" radiative transfer model that uses distributions of T and H₂O, CO₂, O₃, O₂, N₂O, NO₂, and CH₄ amounts as inputs (Crisp et al., 1986)

Chemistry Treatment:

Family Groups (Initially)

Kinetics: Demore et al., 1986

1000Å - 8000Å, Wavelength interval = 50Å

Diurnal Averaging: same as 1-D (Allen et al., 1981)

Cross-sections: DeMore et al. (1986); Allen and Frederick (1982) for O₂ Schumann-Runge Bands;

Froidevaux and Yung (1982) for Herzberg Continuum.

Multiple scattering and albedo treatment same as Froidevaux (1983)

Heterogeneous Removal:

Rainout for soluble species (as in 1-D CIT model)

scattering and cloud albedo using a radiative transfer model described by Sze (1976) and Sze et al. (1981). Heterogeneous removal processes are used to remove H_2O_2 , CH_3OOH , CH_2O , NO_y , Cl_y , Br_x , and F_x in the lowest three layers of the model. Fixed first order loss rates, based on Wofsy (1976), are used to simulate washout and rainout with lifetimes of 5 days, 10 days, and 40 days for levels 1, 2, and 3, respectively.

Integration Algorithm

Concentrations of long-lived atmospheric species are integrated forward in time, with the change in mixing ratio per unit time given by:

$$\frac{\partial f}{\partial t} = -\frac{1}{a \cos \phi} \frac{\partial}{\partial \phi} (f v \cos \phi) - e^{\zeta} \frac{\partial}{\partial \zeta} (f w e^{-\zeta}) + \frac{1}{a^2 \cos \phi} \frac{\partial}{\partial \phi} \left[k_{yy} \cos \phi \frac{\partial f}{\partial \phi} \right] + e^{\zeta} \frac{\partial}{\partial \zeta} \left[k_{zz} e^{-\zeta} \frac{\partial f}{\partial \zeta} \right] + P - Lf$$

where f represents the zonal-mean volume mixing ratio of a trace atmospheric species, v is the horizontal transport velocity, w the vertical transport velocity ($w = d\zeta / dt = -w_e/p_e$), and K_{yy} and K_{zz} are the horizontal and vertical eddy mixing coefficients, respectively. Chemical production and loss is represented by the terms P and Lf , respectively.

The finite differencing scheme used is that developed by Smolarkiewicz (1984). It is a multi-dimensional iterative upstream scheme which removes much of the implicit diffusion of upwind differencing by adding a corrective step to each time step. Negative mixing ratios are not generated provided the time step is small enough. The scheme computes fluxes at grid box boundaries and transports mass only in the direction of fluid flow.

The time step used in the AER model is 12 hours, or 2 steps per day. This yields a CFL parameter of 0.02 or less over most of the model domain, with a maximum value of 0.3 near the upper boundary.

Description of AERI, the Interactive Model

A description of the scheme for calculating the radiative and dynamical variables for the interactive model can be found in "An Evaluation of the Role of Eddy Diffusion in Stratospheric Interactive 2-D Models" by H.R. Schneider, M.K.W. Ko, N.D. Sze, G.Y. Shi, and W.C. Wang, in press, *J. Atmos. Sci.*, 1989.

Section 4.3 CAMBRAL 2-D Model

J.A. Pyle and R.S. Eckman¹
Department of Physical Chemistry
University of Cambridge
Lensfield Road
Cambridge CB2 1EP
UK

Lesley Gray
Rutherford Appleton Laboratory
Chilton, Didcot
Oxon OX1 0QX
UK

UK 2D Eulerian - Mean Circulation Model

Model domain

"pole-to-pole" $\Delta y = \pi/19$

0-60 km (chemistry) $\Delta z = 1/2$ scale height (~ 3.5 km)
0-90 km (dynamics)

$\Delta t = 4$ hours (diurnally averaged)

Dependent variables

Temperature, wind components, chemical constituents

Dynamics

Thermal wind balance is maintained. A second-order partial differential equation solved for the meridional stream function given the forcing by radiative and diabatic heating and eddy heat and momentum fluxes.

Eddy transport of heat and matter employs Reed and German's (1965) diffusion using Luther's (1973) monthly-averaged K's.

Eddy momentum transport derived from satellite data (Crane et al, 1980) above 50 mb and taken from Oort and Rasmussen (1971) below 50 mb.

Rayleigh friction employed to parameterize effect of breaking gravity waves in mesosphere. Friction coefficient is equal to zero below 50 km and rises to 1 day^{-1} at ~ 85 km.

¹ Now at NASA Langley Research Center

Photochemistry

Family grouping as follows-

O(1D), O, O₃
N, NO, NO₂, NO₃, ClONO₂
HO₂NO₂
H, OH, HO₂
Cl, ClO, ClONO₂, HCl, HOCl
CFCl₃
CF₂Cl₂
CCl₄
CH₃Cl
CH₃CCl₃
N₂O₅
CH₄
N₂O
HNO₃
H₂O₂
H₂O

Constant volume mixing ratios above top boundary of photochemical scheme (~60 km).

Reaction rates from DeMore et al. (1987).

Tropospheric rainout rates: first-order removal rates for HNO₃, HCl, HO₂NO₂, and H₂O₂.

Radiation

Curtis matrix method for CO₂ 15μm band.

Cooling to space approximation for O₃ 9.6μm band.

Heating due to absorption of solar radiation by O₂ and O₃. Use solar fluxes from WMO (1981) and absorption cross sections based on WMO (1985) and DeMore et al. (1987).

Infrared cooling and solar heating calculated above 25 km.

Radiative equilibrium or fixed heating rates used from tropopause to 25 km.

Fixed heating rates in troposphere.

References

Harwood and Pyle, 1975, Q.J.R. Met. Soc., 101, 723.
Pyle, 1980, Pageoph, 118, 355.
Gray and Pyle, 1987, Q.J.R. Met. Soc., 113, 635.
Eckman, Haigh, and Pyle, 1987, Nature, 329, 616.

Section 4.4 CAO 2-D Model

V. Philushakin and E. Zhadin
Central Aerological Observatory
U.S.S.R.

The Model of Residual Circulation and the Planetary Waves of the Central Aerological Observatory (U.S.S.R.)

The 2-D residual circulation model of the stratosphere and mesosphere (16-80 km) is similar to the model of Solomon and Garcia (1983), but the IR cooling rates in the 15μ CO_2 and 9.6μ O_3 bands are calculated with parameterization of Fomichev and Shzed (1985). This parameterization takes into account the non-local dependence of the cooling rates upon a temperature profile.

The planetary wave's model calculates non-zonal dynamic and temperature disturbances for the fixed mean flow. The planetary wave sources are the orography and sea-surface temperature contrasts. The dissipation of stationary planetary waves is parameterized by Newtonian cooling and Rayleigh friction. The planetary wave's model (0-80 km) has a high resolution [-0.8° latitude step and -2 km altitude step, $z=\ln(p_0/p)$]. The response of the atmosphere to the sea-surface temperature anomalies can be numerically evaluated by means of the model.

The model of the residual circulation takes into account the planetary wave forcing calculated in the planetary wave's model on the eddy heat and momentum transport by dissipative planetary waves. The eddy heat transport is parameterized in the diffusion form with coefficients which depend upon Newtonian cooling, zonal wind and planetary wave parameters. The dynamical planetary wave effect on the mean flow is calculated in the form of E-P divergence cross-sections. Chemical eddies are calculated as Pyle and Rogers (1980).

Now we create the interactive 3-D model with coupled dynamics and composition of the middle atmosphere. This model will take into account the feedbacks between circulation, thermal regime and composition in a self-consistent manner and will calculate the three-dimensional distribution of the wind, temperature and composition in the stratosphere and mesosphere. The aim of the Central Aerological Observatory 2-D and 3-D models is a numerical study of the anthropogenic and natural effect on ozone layer, the evaluation of stratospheric conditions in the future, and the problem of sudden stratospheric warmings, etc.

Section 4.5 CLKSON 2-D Model

E. Olaguer, H. Yang, and K. K. Tung
Clarkson University¹

Documentation of a Coupled 2-D Model of Dynamics, Radiation and Chemistry in Isentropic Coordinates

Abstract

This is our most recent (Oct. 1988) version of model, with prognostic chemistry. Long-lived species such as O₃, NO_y, CH₄ and N₂O are transported using 2-D circulation deduced from NMC temperature. The isentropic mixing coefficient is determined consistently from the same temperature data. The radiative code has recently been updated, and most of the feedback cycles have now been incorporated.

1. Dynamical Aspects of the Model

The dynamical transport formulation is as given in Tung (1982, 1986), Tung and Yang (1988), and Yang (1988). Briefly, the model is based on a self-consistent non-geostrophic formulation in isentropic coordinates in which the isentropic mixing coefficient is calculated from momentum equation using the same NMC temperature input as that used in the radiative calculations. The vertical coordinate is log (potential temperature) above 350K and log (potential temperature/surface potential temperature) below 350K. The lower surface is currently specified to be at p=1000 mb, but an actual (variable) surface pressure can be easily specified instead, if so desired.

No gravity wave cross-isentrope mixing is incorporated. This limits the applicability of the present version of the model to below the upper stratosphere. No vertical diffusion is included ($K_{zz}=0$) in the present version of the model, although it is recognized that some form of vertical diffusion should be necessary for the troposphere and perhaps also the equatorial lower stratosphere.

The horizontal domain of the model is from pole to pole in increments of 10 degrees of latitude. The vertical domain is from the ground to 8 pressure scale-heights (limited by the availability of NMC temperature data) in increments of about 2.3 km. Resolution is variable and can be increased but at the expense of a considerable increase in computation time.

The Prather scheme (Prather, 1986), as tested and implemented by the Caltech group (Shia et al., 1988) is recently incorporated in place of the scheme of Smolarkiewicz (1983) used in a previous version of the model.

2. The Radiative Transfer Code

The CO₂ IR code utilizes the parameterization developed by Ou and Liou (1983), who employed an empirical broadband emissivity formulation based on the detailed line-by-line calculation of Fels and Schwarzkopf (1981) for the CO₂ 15 micron band.

The O₃ IR scheme is similar to that of Rosenfield et al. (1987). The water vapor scheme consists of an emissivity formulation similar to that employed for CO₂ and is taken from Ramanathan (1976). The water vapor mixing ratio profile may either be specified externally or else take on default values which are determined in the same way as in Rosenfield et al. (1987).

¹Present Affiliation: University of Washington

In the solar radiation part of the code, diurnally averaged heating rates due to solar absorption are computed by the same method employed in the MIT-GIT 3-D model (see Cunnold et al., 1975). Solar declination is not rigorously calculated based on orbital parameters. It is instead computed simply as $\sin \delta = 0.4 \sin(2\pi t/365 \text{ days})$, where $t=0$ on March 21.

There are two versions of the code used to calculate solar absorption by ozone and molecular oxygen: fast and slow. The fast version employs the parameterization of Strobel (1978) as modified by Apruzese et al. (1983) for the absorption of solar radiation in the visible and ultraviolet regions by ozone and molecular oxygen. In addition to the absorption of the direct beam, we include the effects of multiple scattering by the lower atmosphere in the Chappius band. The resulting diffusive radiation is modeled by a pure ozone absorption region on top a reflecting layer with an effective albedo as given by Lacis and Hansen (1974). The ground albedo are taken from Sellers (1965) and are a function of latitude.

The "slow" version of the radiative code employs a more direct calculation of the energy absorption due to ozone and molecular oxygen, and includes the contribution to the atmospheric heating rate by nitrogen dioxide. Multiple scattering is taken into account in a manner similar to that in the "fast" version, except that it is applied to all spectral intervals with wavelengths greater than 3125 Angstroms.

The clear-sky treatment of water vapor absorption in the rear-infrared follows that of Lacis and Hansen (1974).

The treatment of radiation in a cloudy sky is also incorporated in the radiative transfer code.

In addition to radiative transfer, the model also includes the diabatic effects of precipitation in the troposphere. Latent heating is calculated using the approach of Jacqmin and Lindzen (1985) from rainfall data as tabulated by Schutz and Gates (1972a, b) for winter/summer.

3. Photochemistry

A 64-reaction photochemical package is adopted with O_x , NO_x , HO_x , and ClO_x chemistry. The long lived species are advected (and diffused) by model calculated transports, while the short-lived species are calculated algebraically under the assumption of photochemical equilibrium. For the present calculation presented here, the transported species are O_3 , NO_y , CH_4 , and N_2O . The specified species are H_2 , O_2 , N_2 , CO , H_2O , and Cl_y (with an asymptotic value of 2.5 ppbv). All photochemical processes are assumed to take place only in daylight. The interaction involving the species N_2O_5 are ignored. The photodissociation rates are calculated at two solar hour angles as described in section 2 and then averaged. The daylight averaged concentrations of all the constituents are then derived and the 24-hour average odd oxygen generation rate computed by multiplying both the production and loss terms by the fractional length of day.

The required photochemical reaction rate constants, quantum yields, and absorption cross sections are from DeMore et al. (1987), with the exception of cross section for water vapor (from Baulch et al. 1982), ozone and molecular oxygen, which for the Herzberg continuum beyond 200 nm are taken from WMO (1986). The Schumann-Runge O_2 cross sections, on the other hand, are computed as recommended by Allen and Frederick (1982) for wavelengths below 200 nm. The ozone cross sections are those prescribed in WMO (1986) and include the temperature dependence between 260 and 350 nm. Also taken from WMO (1986) are the wave number intervals and photon fluxes used in the computation of the photodissociation rates. For wavelengths beyond 400 nm we use the coarser of the two recommended grids.

The photodissociation rates are calculated assuming that single scattering takes place above the tropopause and multiple scattering below. The Rayleigh single scattering cross sections are taken from WMO (1986). Lower atmosphere effective albedo is computed as in section 2. A Lambert surface is assumed to exist at the ground with the same effective albedo as that of the troposphere. The effects of multiple scattering are included only for wavelengths greater than 321.5 nm.

References:

- Allen and Frederick (1982), JGR, 87, 2066.
Apruzese et al. (1982), JGR, 87, 8951.
Baulch et al. (1982), J. Phys. Chem. Ref. Data, 11, 327.
Cunnold et al. (1975), JAS, 32, 170.
DeMore et al. (1987), Chemical kinetics and photochemical data..., JPL 87-41.
Fels and Schwarzkopf (1981), JGR, 86, 1205.
Jacqmin and Lindzen (1985), JAS, 42, 724.
Lacis and Hansen (1974), JAS, 31, 118.
Ou and Liou (1983), JGR, 88, 5203.
Prather (1986), JGR, 91, 6671.
Ramanathan (1976), JAS, 33, 1330.
Rosenfield et al. (1987), JAS, 44, 859.
Sellers (1965), Physical Climatology, Univ. of Chicago Press, 272 pp.
Schutz and Gates (1972a), Supplemental Global Climatic Data: January, Rand Corp.
Schutz and Gates (1972b), Global Climatic Data for Surface, 800 mb, 400mb: July, Rand Corp.
Shia et al. (1988), submitted to JGR.
Smolarkiewicz (1983), Mon. Wea. Rev., 111, 479.
Strobel (1978), JGR, 83, 6225.
Tung (1982), JAS, 39, 2330.
Tung (1986), JAS, 43, 2600.
Tung and Yang (1988), JGR, in press.
Yang (1988), Numerical Simulation of Global and Antarctic Ozone..., Ph.D. thesis, MIT.
WMO (1986), Atmospheric Ozone 1985: Assessment..., World Meteorological Organization.

Section 4.6 DUPONT 2-D Model

D. Fisher

E.I. DuPont De Nemours & Company, Inc.

General

The present DuPont 2-D atmospheric model is an enhanced version of the model that was extensively described in the paper, Miller et al., Journal of Geophysical Research, Vol 86, p. 12039-12065 (1981). Enhancements have been made to the model as far as treatment of the vertical coordinate system and treatment of the chemistry. Modern recommendations for chemical rate constants are in place.

Model Domain and Resolution

The DuPont 2-D model covers the domain of the entire earth, pole to pole with altitude domain from zero to approximately 56 km. There are ten latitude bins, all of equal areas, parameterized on the sine of latitudes with dimensions of 0.2 units. Therefore bin centers are at $\sin(\phi) = -0.9, -0.7, \dots, 0.9$. There are 18 altitude bins, specified in log-pressure units, each bin corresponding to approximately 3 kilometers.

Transport Treatment Used

Formulation

The transport formulation contains both advective and diffusive terms, in a Lagrangian formulation. In this formulation the circulation is characterized by the sum of the Eulerian mean stream function and an appropriate average of the skew portion of the eddy diffusion tensor. In the Lagrangian formulation only the symmetric portion of the diffusion tensor is needed to define the diffusive transport.

Basis for Winds and Eddy Coefficients

The advective circulation field of Murgatroyd and Singleton (appropriately scaled) is used to approximate the Lagrangian mean flow. The scaling factor of 0.4 was used based on improved atmospheric heating rates determined by Dopplack, which in general are about 1/2 of those employed by Murgatroyd and Singleton in the lower half of the stratosphere.

Below the 15 km lower bound of the Murgatroyd and Singleton velocity field formulation, bounded by constant velocity contours, the vertical component of velocity is calculated using a weighted least squares interpolation procedure including a contour of zero velocity at ground level.

The eddy diffusion parameterization is basically that of Luther (1974) with minor modifications. The latitudinal eddy coefficient K_{yy} has been increased below 10 km to provide a more realistic inter-hemispherical mixing time of 14 months in the troposphere. The vertical eddy coefficient, K_{zz} which represents the most uncertain portion of the Luther parameterization has been replaced by that of Hunten (1975), for all seasons throughout the model stratosphere. This parameterization utilized a tropospheric value of $1.0E+05$ (units = cm^2/sec) and stratospheric values of

$$K_{zz} = 500 * \exp(.10597 * Z)$$

Location of the tropopause and therefore definition of discontinuity in K_{zz} varies with latitude.

Chemistry Treatment Used

Species Computed

The current model utilizes the following species:

Photochemical equilibrium: H, N

Family groups: $O_x = [O(^3P), O(^1D), O_3]$

Active: $H_2O, CH_4, H_2, CO, CH_2O$
 O_x
NO, NO_2 , HNO_3 , N_2O , NO_3 , N_2O_5 , HO_2NO_2
HCl, ClO, Cl, $ClONO_2$, HOCl
 H_2O_2 , OH, HO_2
 $CFCl_3$, CF_2Cl_2 , CCl_4 , CH_3Cl , CH_3CCl_3

(H_2O is only active above 20 km)

Inactive: N_2, O_2, CO_2

Family Grouping (if any)

Calculations are done without major family groupings except odd oxygen (O, O_3).

Diurnal Averaging Scheme

The 'two tank' diurnal averaging scheme is being used for diurnal averaging. The relative sizes of the day and night tanks depend on latitude and season.

Photolysis Calculations

Spectral Resolution

The spectrum is divided into 126 bins to cover wavelengths from 175.4 nm to 730. nm. Bin sizes vary over the spectrum from a coarse size of 10 nm at the high wavelengths to a normal size of 5.0 nm over the middle range. Over the Schumann-Runge portion of the spectrum, the bin size varies in order to capture the features of this region. Bin sizes in this region range from 1.0 to 2.5 nm. Treatment of the Schumann-Runge parallels that of Nicolet and Partimonia.

Source of Cross Section

The cross-sections are from various literature sources:

Photo Reaction	Reference Source
Solar Flux	WMO/NASA 1986
$O_2 \rightarrow 2O$	Nicolet (1980), Frederick and Hudson (1979)
$O_3 \rightarrow O_2 + O$	Gelinas, Relative Quantum Fields from NASA 1049
$\rightarrow O_2 + O(^1D)$	
$NO_2 \rightarrow NO + O$	NASA 1010, NASA Modeling Workshop 1979
$N_2O \rightarrow N_2 + O(^1D)$	Selwyn et al (1977)
$NO \rightarrow N + O$	Frederick and Hudson (1979)
$HNO_3 \rightarrow OH + NO_2$	Johnson and Graham
$H_2O_2 \rightarrow 2OH$	NASA Modeling Workshop, JPL 1982, CIAP
$N_2O_5 \rightarrow NO_2 + NO_3$	Johnson and Graham, NASA 1010
$NO_3 \rightarrow NO + O_2$	
$\rightarrow NO_2 + O$	Magnotta and Johnson (1980)
$HCl \rightarrow H + Cl$	Inn (1976)
$CF_2Cl_2 \rightarrow 2Cl$	JPL 1982
$CFCl_3 \rightarrow 3Cl$	JPL 1982
$CCl_4 \rightarrow 4Cl$	Gelinas
$CHClF_2 \rightarrow Cl$	Watson
$CHCl_2F \rightarrow 2Cl$	JPL 1982
$ClO \rightarrow Cl + O$	Watson (1974)
$HO_2NO_2 \rightarrow OH + NO_3$	Molina and Molina (1980)
O_3 Solar Heating	
O_2 Solar Heating	
$ClONO_2 \rightarrow Cl + NO_3$	NASA 1979 Modeling Workshop
$CH_3Cl \rightarrow Cl$	Robins (1976)
$CO_2 \rightarrow CO + O$	Hudson and Kieffer (CIAP)
$CH_3CCl_3 \rightarrow 3Cl$	Van Laethem-Meuree et al. (1979)
$CH_2O \rightarrow H + HCO$	JPL 1982,
$\rightarrow H_2 + CO$	Interpolated to 230 K
$HOCl \rightarrow OH + Cl$	NASA 1979 Reference Publication
$CH_3O_2H \rightarrow CH_3O + OH$	NASA 1979 Reference Publication
$CH_3O_2NO_2 \rightarrow CH_3O + NO_3$	Cox (1979)

Radiative Transfer Approach

Radiative transfer includes multiple scattering with absorption parameterized based on secant columns of O_2 and O_3 .

Multiple Scattering and Albedo Assumptions

Multiple scattering of solar radiation and ground albedo effects are included in the calculation of photolytic reaction rate constants. For the daytime reaction rates, appropriate averages are taken to account for latitude and season. A Rayleigh phase function is used in the calculations. Ground level albedo is taken as 0.25, independent of latitude and season.

Integration Algorithm Used

Method

The two-dimensional transport and conservation partial differential equations are solved using an appropriate method that removes the numerical dispersion characteristically associated with first order representations of advective transports and also minimized other (discretization) errors produced by the finite grid size. The time-dependent integration of the mass balance equation makes use of an implicit finite difference formula to ensure stability. The specific formulation uses the trapezoidal rule for the transport terms in the mass balance equation, and the backward Euler's approximation for the chemical production and loss terms. At each time step, the finite difference formula is solved for the mixing ratio of each species at each grid point by using a Newton-Raphson iteration scheme until convergence is achieved. The calculations are preformed on DuPont's CRAY-1 computer.

Time Step

For most runs, a time step of 1/60th of a season is used or about 18 hours.

Treatment of Negative Mixing Ratios

Negative mixing ratios are not encountered in normal runs.

Heterogeneous Removal Processes

Species Removed: The following species are removed via rainout below 10 km with a 5 day time constant.

Cl	OH
ClO	HO ₂
ClONO ₂	H ₂ O ₂
HCl	NO ₂
HNO ₃	#CH ₃ O ₂
CH ₂ O	#CH ₃ O ₂ H
HOCl#CH ₃ O ₂ NO ₂	
HO ₂ NO ₂	
OCIO	

. # Normally set to zero.

Basis for Removal Rate

This rain-out time constant was derived by fitting a first order equation to the tropospheric water vapor data and evaluating the time constant. Also sensitivity analyses were run to determine that the net effect is not extremely sensitive to the precise value of this constant.

Section 4.7 GISS 1-D and 3-D Models

M.J. Prather
Goddard Institute for Space Studies

GISS 1-D Photochemical Model

JPL 87 (cross-sections, kinetics, fluxes, temp dep of O₃ not N₂O₅)

- radiation code uses multi-stream scattering & spherical solar source
- S-R bands & NO by opacity distribution function (ODF: Fang et al, Harvard) updated to include temperature dependence of ODF
- calculations use the January mean profiles for O₃ and T as specified
- latitude grid is 85S (10 deg) 85N (18 latitudes)
- altitude grid is pressure-height $z^* = 16 \log_{10}(1000/p)$ begin 0 (2 km) 62 km (32 levels)

GISS: 3-D Chemical Tracer Model

Michael J. Prather (GISS)
Maria M. Garcia (Columbia U.)
David Rind (GISS)
2880 Broadway
New York, NY 10025

The chemical tracer model (CTM) uses the winds and convection from the GISS general circulation model (GCM) for the middle atmosphere. The GCM stores horizontal mass fluxes across the boundary of grid boxes and surface pressures at 4-hour intervals. The CTM is run from these history tapes. The coordinates of the CTM are the same as the GCM:

- Sigma coordinates in layers 1-9 (984 mb-100 mb)
- fixed-pressure in layers 10-23 (100 mb, 46 mb, 22 mb,...)
- 3 levels per decade in pressure
- 7.83 deg lat boundaries = (90S, 82.17S, 74.35S,..., 3.91S, 0, 3.91N, 7.8N..., 82.17N, 90N)
- 10 deg long
- Total 23 layers x 24 lat x 36 long.

The 3-D tracer continuity equation is solved by operator splitting: advection of tracer is done upstream with second-order moments. Diffusion and convective mixing only in the troposphere; chemistry every 4 hours (diurnal average only). Chemistry is limited to a single tracer with linearized production and loss. The photochemical model assumes observed ozone climatologies and temperature to calculate zonal and monthly averaged chemistry. Ozone chemistry is fully linearized, other gases (N₂O, CFCl₃, CF₂Cl₂) use linear loss frequencies from tables (24 lat x 13 alt x 12 months).

References

- Prather, M.: Numerical advection by conservation of second-order moments, J. Geophys. Res., **91**, no. D6, 6671-6681, May 1986.
- Prather, M.; McElroy, M. Wofsy, S.; Russell, G.; Rind, D.; Chemistry of the global troposphere: fluorocarbons as tracers of air motions, J. Geophys. Res., **92**, no. D6, 6579-6613, June 1986.
- Rind D.; Suozzo, R.; Balachandran, N.K.; Lacis A.; Russell G.; The GISS global climate-middle atmosphere model. Part I: model structure and climatology, J. Atmos. Sci., **45**, 330-370, 1988.
- Part II: Model variability due to interactions between planetary waves, the mean circulation and gravity wave drag. J. Atmos. Sci., **45**, 371-386, 1988.

Section 4.8 GSFC1 2-D Model

P.D. Guthrie, C.H. Jackman and T.L. Kucsera
Goddard Space Flight Center

Domain, Resolution, and Timestep

85°S to 85°N, 10° latitude bands

Ground to -60 km altitude with -2 km vertical resolution
(log pressure coordinates)

Chemistry

35 species computed, all transported independently (no families)

Diurnal averaging based on square wave approximation, day/night ratios scaled to 1-D mid-latitude model.

Photolysis calculations -

Spectral resolution - 39 wavelength intervals

In Angstroms -1215.67, 1700-1724, 1724-1739, 1739-1754, 1754-1770, 1770-1786, 1786-1801, 1802-1818, 1818-1835, 1835-1852, 1852-1869, 1869-1887, 1887-1905, 1905-1923, 1923-1942, 1942-1961, 1961-1980, 1980-2000, 2000-2020, 2020-2105, 2105-2198, 2198-2299, 2299-2410, 2410-2532, 2532-2667, 2667-2817, 2817-2857, 2857-2985, 2985-3030, 3030-3077, 3077-3125, 3125-3175, 3175-3225, 3225-2275, 3375-3575, 3575-3775, 3775-3975, 3975-5475, 5475-7350

Source of cross sections used - World Meteorological Organization, Atmospheric Ozone 1985
Exception is O₂ - Allen and Frederick (1982) for Schumann Runge bands, Herman and Mentall (1982) for Herzberg continuum.

Radiative transfer approach - Two-stream radiative transfer method of Herman (1979) which is based on the matrix operator method of Plass et al. (1973)

Multiple scattering and albedo assumptions - Two-stream approach with 0.3 assumed as albedo at ground for all wavelengths.

Integration Algorithm

Alternative direction forward time differences ("angled derivative").

Fourth order spatial differences centered in the interior shifting to one-sided at the boundaries.

Newton-Raphson interactive solution of species continuity equations.

Time step is one day, decreasing if needed.

Time step reduced if negative mixing ratios occur.

Heterogeneous Removal

"Solubles" removed at rate proportional to specified "Rain" profile (HNO_3 , HCl , H_2O_2 , NO , CH_2O , CH_3OOH)

Transport Treatment

Residual mean formulation

Base case winds, based on Rosenfield et al. heating calculations (in turn based on NMC temperature data, SBUV ozone, present-day CO_2)

Water vapor: 3.2 ppm above 20 mb, fixed relative humidity (Manabe and Wetherald) in troposphere

Base eddy coefficients

Stratosphere	$K_{yy} = 2 \times 10^9 \text{ cm}^2\text{-s}^{-1}$
	$K_{zz} = 2 \times 10^3 \text{ cm}^2\text{-s}^{-1}$
Troposphere	$K_{yy} = 2 \times 10^{10} \text{ cm}^2\text{-s}^{-1}$
	$K_{zz} = 2 \times 10^4 \text{ cm}^2\text{-s}^{-1}$
transition zone between 500-100 mbar	

Section 4.9 GSFC2 2-D Model

C.H. Jackman, A.R. Douglass, R.S. Stolarski and P.D. Guthrie
Goddard Space Flight Center

Summary of the NASA/GSFC Fast 2-D Model

GSFC2, a two-dimensional (2-D) residual circulation stratospheric model, was developed to be used as a tool for examining the sensitivity of model calculations to photochemical and dynamical inputs and assumptions and evaluating the response of stratospheric ozone to a wide range of possible scenarios for changes in trace gases. Photochemical inputs include the reaction rates, photodissociation cross sections, solar flux values, and solar cycle effects, including both solar flux variations and particle precipitation events. Dynamical inputs include the diffusion coefficients, the circulation, and their seasonal and inter-annual variability. Currently the model is non-interactive between ozone and dynamics; the dynamics are changed monthly and computed from observed temperature and ozone.

To be useful for such a wide range of applications, the model was designed to require minimal computer resources. Family chemistry approximations are used to reduce the number of species continuity equations that must be solved. The species continuity equations are solved through process splitting, that is by successive application of the advection, diffusion and photochemical operators. The advection is calculated using an efficient non-dispersive transport scheme developed by Prather (1986). The diffusion operators act on the transported fields. The photochemical production and loss are calculated using the previous timestep's values for species concentrations; this implicitly assumes that the timestep to timestep changes in species concentration are small. The main inputs to this model are summarized in the accompanying table on the following pages:

More detailed information about GSFC2 can be obtained by calling or writing:

C.H. Jackman	A.R. Douglass
Code 616	Code 616
NASA/GSFC	NASA/GSFC
Greenbelt, MD 20771	Greenbelt, MD 20771
phone (301) 286-8399	phone (301) 286-2337
or FTS 888-8399	or FTS 888-2337

Domain, Resolution, and Timestep

85°S to 85°N, 10° latitude bands
Ground to -60 km altitude with -2 km vertical resolution (log pressure coordinates)
One day timestep - 360 day model year
Photolysis rates computed every 10 days
Residual circulation, K_{yy} 's and K_{zz} 's computed every 30 days
Species are output in daytime average form

Transported Families

O_x
Odd N

Cl_x

Derived Species

O_3 , $O(^3P)$, $O(^1D)$
N, NO, NO_2 , NO_3 , $2N_2O_5$
 HNO_3 , HO_2NO_2 , $ClONO_2$
Cl, ClO, HOCl, $ClONO_2$, HCl

Transported Species

N₂O, H₂, CH₄, CCl₄, CH₃Cl, ClFCl, CF₂Cl₂, CH₃CCl₃, CH₃OOH, CO

Photochemical Species

H, OH, HO₂, H₂O₂, HCO, CH₂O, CH₃O, CH₃O₂

Dissociation Rates

Spectral Resolution

Reference or Explanation

39 wavelength intervals

Solar Flux

WMO (1986)

Diurnal Averaging

Look up table for diurnal average solar flux as function of optical depth, latitude, and solar declination.

Table produced by detailed diurnal cycle calculations using a 1D photochemical model (Herman 1979).

Multiple Scattering

Two-stream radiative transfer (Herman, 1979)

Albedo

0.3 at ground for all wavelengths:
no clouds included

Cross Sections

JPL 87-41

O₂, NO

Allen and Frederick (1982)

Reaction Rates

From JPL 87-41

Heterogeneous Removal

HNO₃, HO₂NO₂, HCl, H₂O₂, and CH₃OOH rained out in troposphere

Dynamical Inputs

Reference or Explanation

Residual Circulation

Dunkerton (1978)

Heating Rates

Rosenfield et al. (1987), p<100mbar
Doplick (1974, 1979), p>100 mbar

Temperature

NMC data, 4 year monthly average

Diffusion

K_{yy}, K_{yz}

Stratosphere: Newman et al. (1988)

Troposphere: $1 \times 10^{10} \text{ cm}^2/\text{sec}$ at ground, decreasing with altitude to stratosphere value

K_{zz}

Stratosphere: $2 \times 10^3 \text{ cm}^2/\text{sec}$

Troposphere: $1 \times 10^4 \text{ cm}^2/\text{sec}$ at ground, decreasing with altitude to stratospheric value

Boundary Conditions

Value

Top

Zero flux for all transported families and species

Bottom

O_x

Deposition velocity - 0.1 cm/sec

Odd N

Fixed mixing ratio - 100 pptv

Cl_x

Zero flux

N_2O

Fixed mixing ratio - 300 ppbv

H_2

Fixed mixing ratio - 0.5 ppmv

CH_4

Fixed mixing ratio - 1.6 ppmv

CCl_4

Fixed mixing ratio - 100 pptv

CH_3Cl

Fixed mixing ratio - 700 pptv

CFCl_3

Fixed mixing ratio - 170 pptv

CF_2Cl_2

Fixed mixing ratio - 285 pptv

CH_3CCl_3

Fixed mixing ratio - 100 pptv

CH_3OOH

Zero Flux

CO

Fixed mixing ratio - 100 ppbv

Section 4.10 LARC 3-D Model

W. Grose, R. Eckman, R. Turner, and T. Blackshear
NASA Langley Research Center
Mail Stop 401B
Hampton, VA 23665-5225

NASA Langley 3-D GCM/Chemistry Model

Model Domain	pole-to-pole with 32 latitude bins at approximately 5 degree intervals 0-60 km with 12 height intervals using sigma coordinates time step = 30 minutes
Dependent variables	temperature, wind components, chemical constituents chemistry/transport done "off-line"
Dynamics	Spectral, primitive equation, general cir- culation model to zonal wave number 16 with triangular truncation
Chemistry	Family approach with six families/species explicitly integrated: O_x , NO_y , HNO_3 , Cl_x , N_2O_5 , H_2O_2 39 species partitioned using 115 reactions
Radiation	Shortwave radiation: method of Lacis and Hansen (1974) Longwave radiation: Newtonian approx- imation
References	Grose, W.L., J.E. Nealy, R.E. Turner, and W.T. Blackshear, Modeling the transport of chemically active constituents in the stratosphere, Proceedings of the NATO Erice Workshop, 1987. Blackshear, W.T., W.L. Grose, and R.E. Turner, Simulating sudden stratospheric warming synoptic evolution, <u>Quart. J. Roy. Met. Soc.</u> , <u>113</u> , 815-846, 1987.

Section 4.11 LLNL 2-D Model

D.J. Wuebbles, P.S. Connell, K.E. Grant, and R. Tarp
Lawrence Livermore National Laboratory

The LLNL zonally-averaged two-dimensional chemical-radiative transport model currently determines the atmospheric distributions of 31 chemically active atmospheric trace constituents in the troposphere and stratosphere. The model domain extends from pole to pole, and from the ground to 0.56 mb (approximately 0 to 54 km). The sine of latitude is used as the horizontal coordinate because of its advantages in the transformed continuity equation, with uneven increments corresponding to about 10° in latitude used to provide adequate resolution, particularly towards the poles. The vertical coordinate corresponds to the natural logarithm of pressure ($z^* = -H_0 \ln(p/p_0)$), where H_0 is the assumed scale height of 7.2 km, and p_0 is the surface pressure, 1013 mb). The vertical resolution is $\ln(p/p_0) = 0.417$ or approximately 3 km.

Approximately 95 chemical and photochemical reactions are included in the model. Reaction rates, solar flux data, absorption cross-sections, and quantum yields are based on the latest NASA panel recommendations (JPL 87-41, 1987). Photodissociation rates, including the effects of multiple scattering, are computed as a function of time at each zone, with optical depths consistent with calculated species distributions.

The diabatic circulation for the ambient atmosphere is determined using net heating rates calculated in an internally consistent way with the derived species distributions. The technique for deriving the diabatic circulation is similar to that used by Solomon et al. (1986): the vertical velocity is determined from the zonally averaged residual Eulerian thermodynamic equation, while the horizontal velocity is determined using the equation for mass continuity.

The net heating rates are determined using accurate solar and infrared radiative models. The solar model includes absorption and scattering effects for O_3 , O_2 , and NO_2 at ultraviolet and visible wavelengths, and for H_2O , CO_2 , and O_2 in the near infrared. The longwave emission and absorption by O_3 , CO_2 , and H_2O are included in the infrared sub-model.

Temperatures for the ambient atmosphere vary continuously, over the annual cycle, based on the reference model of Barnett and Corney (1985). The derived diabatic circulation depends strongly on the temperature distribution; by using observed temperatures for the ambient atmosphere, a more accurate representation of the diabatic circulation can be derived. The model determined net radiative heating rates and resulting diabatic circulation compare well with those derived from LIMS data (Kiehl and Solomon, 1986; Rosenfield et al.; 1987; Solomon et al.; 1986).

For the perturbed atmosphere, a perturbation form of the thermodynamic equation is solved for the changes in stratospheric temperatures resulting from changes in the distributions of ozone and other radiatively active constituents. Using this approach, the diabatic circulation is assumed to be unchanged in the perturbed atmosphere from that calculated for the ambient.

Turbulent eddy transport is parameterized through diffusion coefficients K_{yy} and K_{zz} . In the current version of the model, a value K_{yy} of $2 \times 10^9 \text{ cm}^2 \text{ s}^{-1}$ is assumed at all stratospheric altitudes and latitudes, and values of 1×10^{11} in the troposphere. Values of K_{zz} are $1 \times 10^3 \text{ cm}^2 \text{ s}^{-1}$ in the lower stratosphere, increasing slowly with altitude based on gravity wave modeling studies.

The continuity equation for each individual species is solved using a variable time step, variable order, implicit technique for solving stiff numerical systems with strict error control. Advection terms are treated accurately using the two-dimensional transport algorithm of Smolarkiewicz (1984). The diurnal-averaged concentrations for each species at each zone are calculated at each time step. Accurate diurnal calculations are used to derive time-varying factors for each chemical and photochemical reaction included in the diurnal-averaged version of the model.

Section 4.12 MPIC 2-D Model

C. Bruehl and P.J. Crutzen
Max Planck Institute for Chemistry, D-6500
Federal Republic of Germany

2-D Mainz Chemistry - Climate - Model

Grid	10° latitude, surface to 54 (60) km pressure grid, resolution about 2 km
Chemistry	families including Br _x , about 140 reactions, timestep 2 hrs.
Transport	Eulerian, large K _{yy} , K _{yz} and K _{zz} , Circulation from Louis, 1974. In development: Circulation from our radiation code (diabatic).
Radiation	UV+ VIS Delta two-stream method, 176 spectral intervals, clouds included. Includes IR broadband-model of Ramanathan (CO ₂ Kiehl, Ram., 1983). In present version the radiation is not used for calculation of temperatures or circulation.
References	Gidel et al (1983): <u>J. Geophys Res.</u> 88 , 6622. Bruehl, Crutzen (1988): Climate Dynamics, 2, 173.
Contact	Ch. Bruehl 49-6131-305434 Bitnet CHB@DGAIPP1S Fax - 305388

Section 4.13 MRI 2-D Model

Toru Sasaki
Meterological Research Institute
1-1 Nagamine, Tsukuba, Ibaraki,
305 Japan

The present version of MRI 2-D photochemical model calculates the mixing ratio of minor constituents with prescribed temperature, circulation and eddy diffusion coefficients. The basic equation of the model is

$$\frac{\partial \bar{f}_x}{\partial t} + \frac{1}{a \cos \phi} \frac{\partial (\bar{f}_x \bar{v} \cos \phi)}{\partial \phi} + e^{\xi} \frac{\partial (e^{-\xi} \bar{f}_x \bar{w})}{\partial \xi} = \frac{\bar{Q}_x}{N} + \bar{F}_x$$

where \bar{f}_x is the mixing ratio of constituent x , ϕ is latitude, $\xi = -\ln(p/p_0)$ is altitude, v and w are northward and upward velocity of the circulation, respectively, Q_x is photochemical production, F_x is eddy diffusion transport, a is the earth radius and N is the number density of the air. The overbar — denotes its diurnal or zonal mean.

Grid points are defined as follows. The latitudinal range is divided into 18 divisions of 10° width from the south pole to the north pole and the altitude range ($\xi = 0$ to 8) is divided into 16 divisions of $\Delta \xi = 0.5$ height. So we get 18×16 cells in the model meridional plane. Mixing ratio, temperature, photochemical production, etc., are defined at the center point of each cell, v and w are defined at the center point of the vertical and horizontal wall, respectively, and eddy diffusion coefficients are defined at the cross point of the walls. So we can calculate mixing ratio of minor constituents from 85° S to 85° N and from $\xi = 0.25$ to 7.75.

We include 38 species in the model, and the mixing ratio of 36 species are calculated. Some species, which are photochemically active and quickly converted into each other, are grouped as a family. Each of these families is treated as one constituent in the basic equation. The mixing ratio of each species of the family is determined on the photochemical equilibrium condition. The species and the families are as follows:

$O_x (=O_3+O+O(^1D))$,
 N_2O , $NO_x (=N+NO+NO_2)$, NO_3 , N_2O_5 , HNO_3 , HNO_4 ,
 H_2O , H_2 , $HO_x (=H+OH+HO_2)$, H_2O_2 ,
 CH_4 , $CHO_{x1} (=CH_3+CH_3O_2)$, CH_3O_2H , $CHO_{x2} (=CHO+CH_2O+CHO)$, CO , CO_2 ,
 CF_2Cl_2 , $CFCl_3$, CCl_4 , CH_3Cl , CH_3CCl_3 , $ClO_x (=Cl+ClO)$, HCl , $HOCl$, $ClONO_2$.

We set some boundary conditions in the model. The boundary mixing ratio is given at the surface ($\xi = 0$), it affects the above atmosphere by diffusion. Some species are removed by rainout in the first and second layer with 10 days lifetime.

We consider 83 chemical reactions and 31 photodissociations in the model. The kinetic data and the absorption cross sections are from JPL 87-41. Solar flux at the top of the atmosphere and the absorption cross sections of O_2 and O_3 are from WMO (1986).

The data of temperature is from Louis (1975) and circulation is from Murgatroyd and Singleton (1961) multiplied by 0.5. The eddy diffusion coefficients are selected by trial and error to simulate ozone and other trace species well. In our model the components of the eddy diffusion coefficients are formulated by

$$\begin{aligned}
K_{yy} &= K_{yy0}(\xi) + A(\xi) \cdot B(\phi) \cdot C(s) \\
K_{yz} &= A(\xi) \cdot B(\phi) \cdot C(s) \cdot D(h) \\
K_{zz} &= K_{zz0}(\xi) + A(\xi) \cdot B(\phi) \cdot C(s) \cdot D(h) \cdot D(h).
\end{aligned}$$

$K_{yy0}(\xi)$ is set to be $(50 \rightarrow 10) \times 10^9 \text{ cm}^2 \text{ sec}^{-1}$ for $0 < \xi < 2$ and $2 \times 10^9 \text{ cm}^2 \text{ sec}^{-1}$ for $\xi > 3$. $K_{zz0}(\xi)$ is set to be $(150 \rightarrow 20) \times 10^3 \text{ cm}^2 \text{ sec}^{-1}$ for $0 < \xi < 2$, $(2 \rightarrow 6) \times 10^3 \text{ cm}^2 \text{ sec}^{-1}$ for $3 < \xi < 5$, and $25 \times 10^3 \text{ cm}^2 \text{ sec}^{-1}$ for $\xi > 6$. The other terms are seasonal contributions from planetary wave activity. $A(x)$ is an altitudinal factor to be 1 for lower to middle stratosphere and to be 0 otherwise. $B(\phi)$ is a latitudinal factor set to be 1 for midlatitude and to be zero otherwise. $C(s)$ is a seasonal function of wave activity parameter set to be $9 \times 10^9 \text{ cm}^2 \text{ sec}^{-1}$ for winter and 0 for summer. $D(h)$ is declination set to be 8×10^{-4} for southern and -8×10^{-4} for northern hemisphere.

Our model year has 360 days. Prescribed seasonal data such as temperature, circulation and eddy diffusion coefficients are renewed by every 3 days by interpolation. For the assessment of diurnal change effects diurnal change of density and photodissociation rates are calculated by every 15 days. A time step of diurnal change calculation is 10 minutes. From these calculations we define diurnal change coefficients as,

$$e_{kl} = \overline{N_k \cdot N_l} / (\bar{N}_k \cdot \bar{N}_l)$$

$$e_j = \overline{J_j \cdot N_j} / (\bar{J}_j \cdot \bar{N}_j)$$

where N_k is number density of the species k , J_j is the j -th photodissociation rate as a function of local time. Using these coefficients we can easily obtain diurnal mean photochemical production by diurnal mean value of density and photodissociation rate, i.e.,

$$\bar{Q}_x = \pm \sum e_{kl} \cdot \bar{R}_{kl} \cdot \bar{N}_k \cdot \bar{N}_l \pm \sum e_j \cdot \bar{J}_j \cdot \bar{N}_j$$

So we can predict the zonal mean mixing ratio of the next time step on the basis of the present zonal mean value.

A time step of the zonal mean calculation is 8 hours. When the photochemical lifetime gets less than a time step, numerical instability generates. To avoid the instability some relaxation method of the change rate is introduced. To assure mass conservation the excess or the lack caused by relaxation is compensated by its converted species.

This method enables us to execute the stable integration on any photochemical condition.

References

- JPL 87-41 (W.B.DeMore et al.), Chemical Kinetics and Photochemical Data for Use in Stratospheric Modeling, Evaluation 8, JPL Pasadena, 1987.
 Louis, J.J., Mean Meridional Circulation. The Natural Stratosphere of 1974, in CIAP Monograph, U.S. Dept. of Transportation, 6-23, 1975.
 Murgatroyd, R.J., and F. Singleton, Possible Meridional Circulations in the Stratosphere, Quart. J. Roy. Meteorol. Soc., 87, 125-135, 1961.
 W.M.O., Atmospheric Ozone 1985, Assessment of Our Understanding of the Proceedings Controlling Its Present Distribution and Change, Geneva, 1986.

Section 4.14 NOCAR 2-D Model

R.R. Garcia, S. Solomon, and J.T. Kiehl
National Oceanic and Atmospheric Administration
National Center for Atmospheric Research

Garcia - Solomon - Kiehl 2-D Model

The model used for stratospheric studies extends from 100 mb (about 16 km) to 0.04 mb (about 70 km), and from 89.5 S to 89.5 N.

Dynamics:

The transport is represented by the residual Eulerian circulation computed from the mean residual streamfunction χ^* . The streamfunction equation includes nonlinear terms, and a specification of χ^* at the lower boundary. The temperature field is obtained from the thermodynamic equation given the residual Eulerian velocities v^* and w^* . The mean zonal wind is evaluated from the temperature field assuming thermal wind balance. Rayleigh friction is prescribed as a function of height only. Eddy diffusion coefficients are non-interactive and are presented as indicated in the archived model results. See Garcia and Solomon (1983), Solomon et al. (1985) for details.

Photochemistry:

Continuity equations including transport terms are solved for the following species:

$O_x (=O(^1D) + O(^3P) + O_3)$
 $HO_x (=OH + HO_2 + H)$
 $NO_x (=NO + NO_2 + NO_3 + 2N_2O_5)$
 HNO_3
 H_2O_2
 $ClO_x (=Cl + ClO + HOCl + ClONO_2)$
 HCl
 CF_2Cl_2
 $CFCl_3$
 CCl_4
 CH_3Cl
 H_2O
 CH_4
 N_2O
 H_2

The O_x , HO_x , NO_x , and ClO_x chemical families are partitioned based on steady-state approximations when the time scale for partitioning is less than 10 minutes. Longer-lived individual members of these chemical families (e.g., N_2O_5 at high latitudes) are solved for individually, including transport terms, whenever their photochemical lifetimes exceed 10 minutes.

CH_4 oxidation chemistry is considered in detail, and includes the chemistry of relevant intermediates such as H_2CO , HCO , etc., as described by LeTexier et al. (1988).

Approximation number 4 of Cogley and Borucki (1976) is used to derive daytime averaged photolysis

rates. These values are applied to all photolysis reactions during the sunlit period of the day at any particular latitude. Photolysis rates are set to zero at night, so that this essentially corresponds to a "two-tank" approximation.

See also Garcia and Solomon (1983), Solomon and Garcia (1983; 1984), and Solomon et al. (1985).

Radiation:

Heating due to absorption of ultraviolet and visible radiation by ozone, molecular oxygen, and NO_2 is evaluated using the same wavelength intervals as those employed in the photolysis calculations. Near-infrared heating by CO_2 and water vapor employs the solar radiation code used in the NCAR Community Climate Model (Kiehl et al., 1987).

The longwave cooling rates due to CO_2 , O_3 , and H_2O are obtained from the computed mixing ratios and temperature. Longwave radiative cooling is calculated with the radiation model from the NCAR CCM. The scheme is based on the broadband absorption method (see Kiehl et al., 1987). CO_2 and O_3 cooling include Voigt line effects as described by Kiehl and Briegleb (1988).

References:

- Cogley, A. C. and W. J. Borucki, Exponential approximation for daily average solar heating and photolysis, J. Atmos. Sci., **33**, 1347, 1976.
- Garcia, R. R. and S. Solomon, A numerical model of the zonally average dynamical and chemical structure of the middle atmosphere, J. Geophys. Res., **88**, 1379, 1983.
- Kiehl, J. T., R. J. Wolski, B. P. Briegleb, and V. Ramanathan, Documentation of radiation and cloud routines in the NCAR Community Climate Model (CCM1), NCAR Technical Note, NCAR/TN-288+IA, 1987.
- Kiehl, J. T. and B. Briegleb, A new parameterization of the absorptance due to the 15 μm band system of carbon dioxide, submitted to J. Geophys. Res., 1988.
- LeTexier, H., S. Solomon, and R. R. Garcia, The role of molecular hydrogen and methane oxidation in the water vapor budget of the stratosphere, Quart. J. Roy. Met. Soc., **114**, 281, 1988.
- Solomon, S. and R. R. Garcia, On the distribution of nitrogen dioxide in the high latitude stratosphere, J. Geophys. Res., **88**, 5497, 1983.
- Solomon, S. and R. R. Garcia, On the distribution of long-lived tracers and chlorine species in the middle atmosphere, J. Geophys. Res., **89**, 11633, 1984.
- Solomon, S., R. R. Garcia, and F. Stordal, Transport processes and ozone perturbations, J. Geophys. Res., **90**, 12981, 1985.

Section 4.15 OSLO 2-D Model

I.S.A. Isaksen and F. Stordal
University of Oslo
Institute of Geophysics
P.O. Box 1022 Blindern
0315 Oslo
NORWAY

* Brief:

A two dimensional transport-chemistry model of the troposphere and the stratosphere (0-50 km), covering latitudes from pole to pole, employing the diabatic circulation with small eddy diffusion coefficients in the stratosphere.

*Journal reference for model documentation:

Stordal, F., Isaksen, I.S. A. and Horntveth, K. 1985. A diabatic circulation two-dimensional model with photochemistry: Simulations of ozone and long-lived tracers with surface sources, J. Geophys. Res., 90, 5757-5776.

Isaksen, I.S.A. and Stordal, F. 1986. Ozone perturbations by enhanced levels of CFCs, N_2O and CH_4 : a two-dimensional diabatic circulation study including uncertainty estimates. J. Geophys. Res., 91, 5245-5263.

Stordal, F. and Isaksen, I.S.A. 1987. Ozone perturbations due to increase in N_2O , CH_4 and chlorocarbons: two-dimensional time dependent calculations, Tellus, 39B, 333-353.

*Units:

Gas concentrations given as volume mixing ratios
Heating rates given in K/day

*Time steps covered:

Mid-month data twelve months of year 1980.

Section 4.16 WISCAR 2-D Model

G. Brasseur, M.H. Hitchman, and A. DeRudder
University of Wisconsin and
National Center for Atmospheric Research

This radiative-chemical-dynamical model was designed at the Belgian Institute for Space Aeronomy (BISA) by G. Brasseur, M. Dymek, and K.E. Falise and further developed at NCAR. Two cooperative projects have been established for mutual benefit. A detailed radiative code has been provided by Drs. P. Crutzen and C. Bruhl of the Max Planck Institute for Chemistry in Mainz, Germany. A transport scheme is being developed by Dr. M. Pirre of the Laboratory for Physics and Chemistry of the Environment in Orleans, France. It will be expressed in isentropic coordinates but will retain the same chemical and radiative codes.

1. Model domain and resolution

0-85 km $\Delta = 1$ km
pole-pole $\Delta = 5^\circ$

2. Transport treatment

Entropy and chemical species are advected by a residual (transformed Eulerian) mean meridional circulation in log-pressure coordinates. The residual mean meridional stream-function is forced by spatial gradients in wave driving and in radiative heating or cooling (see Garcia and Solomon, 1983). Zonal winds are derived from the thermal wind law and a seasonally-varying surface boundary condition. The zonal wind distribution determines the distribution of wave driving and vertical eddy diffusivity due to gravity waves and of wave driving and meridional eddy diffusivity due to Rossby waves. These self-determined eddy diffusivities are used with the residual circulation and photochemical sources and sinks to determine distributions.

Two codes are available for radiative heating and cooling calculations: fast or accurate. For fast calculations IR transfer is approximated by a Newtonian relaxation toward a seasonally-varying climatological temperature cross-section, while the parameterization of Schoeberl and Strobel (1978) is used for isolation absorption by ozone. The detailed code was provided by Crutzen and Bruhl who adapted an earlier model of Ramanathan. IR transfer is calculated for carbon dioxide, ozone, water vapor, methane, nitrous oxide, and CFC-11 and CFC-12. Solar heating is calculated for ozone, nitrogen dioxide, water vapor, and carbon dioxide.

The model can be run with a variety of dynamical forcings. Most simply, momentum drag is parameterized by a Rayleigh friction and eddy diffusivities vary with altitude only. A more complex representation of the effects of small scale eddies is afforded by the breaking gravity wave parameterization of Lindzen (1981) and Holton (1982). A spectrum of phase speeds were chosen and parameters were tuned to yield residual circulations comparable to those inferred from LIMS observations (Hitchman and Leovy, 1986). A new parameterization of Rossby wave driving was introduced to provide a self-consistent determination of their torque on the zonal flow and dispersion of tracers (Hitchman and Brasseur, 1987). A conservation equation for Rossby wave action is solved, given climatologically-varying upward fluxes across the tropopause and a damping profile. The meridional eddy diffusivity and zonal torque are proportional to the flux convergence of wave action. A background value of $3 \times 10^5 \text{ m}^2/\text{s}$ is added to the calculated meridional eddy diffusivity.

3. Chemistry Treatment

Approximately 40 species are included. The family grouping method is used. A discrimination is made between (1) long-lived species and families and (2) short-lived species. The source gases are: N_2O , CCl_4 , CFCl_3 , CF_2Cl_2 , CH_3CCl_3 , CH_3Cl , CH_4 , C_2H_2 , C_2H_6 , C_3H_8 , HCN , CH_3CN , H_2O , H_2 , and CO_2 . Transported families include NO_y ($\text{N} + \text{NO} + \text{NO}_2 + \text{NO}_3 + 2\text{N}_2\text{O}_5 + \text{HNO}_3 + \text{HO}_2\text{NO}_2 + \text{ClONO}_2$), Cl_x ($\text{Cl} + \text{ClO} + \text{HCl} + \text{HOCl} + \text{ClONO}_2$), and O_x ($\text{O}_3 + \text{O}(^3\text{P}) + \text{O}(^1\text{D})$). Long-lived (transported) species are: CO , HNO_3 , N_2O_5 , and H . Short-lived species include: $\text{O}(^1\text{D})$, $\text{O}(^3\text{P})$, O_3 ; N , NO , NO_2 , NO_3 , HNO_4 ; Cl , ClO , HCl , ClONO_2 , HOCl ; OH , HO_2 , and CH_3O_2 . The reaction rate constants JPL (1985) compilation.

4. Photolysis Calculations

Photodissociation coefficients (J 's) are calculated by spectral integration, using the 171 wavelength intervals specified by Ackerman (1971). These correspond to a resolution of 500 cm^{-1} (wavenumber) between 117 and 308 nm, of 2.5 nm (wavelength) between 310 and 645 nm, and of 5 nm between 650 and 730 nm. The solar spectrum is specified according to Brasseur and Simon (1981). The cross sections are taken from the model used at BISA and are close to the values given in the JPL compilation.

Different routines for the calculation of the photodissociation coefficients are available in the code. The most comprehensive method includes multiple scattering and albedo, and is based on formalism of Fred Luther (private communication): six orders of scattering are considered together with absorption by O_2 and O_3 . The surface albedo has to be specified. Penetration of solar ultraviolet in the Schumann-Runge bands is calculated by the parameterization of either Kockarts (1976) or of Nicolet and Peetermans (1980). For photolysis of NO in the δ (0-0) and δ (1-0) bands, the parameterization by Nicolet (1979) is used. The model can also be run using less detailed but faster codes for the calculation of the J 's.

The diurnal average of the photodissociation coefficients is approximated by a 4 point integral between sunrise and sunset (see Cunnold et al., 1975). This procedure allows us to calculate an accurate mean J for different altitudes, latitudes and season with minimum computer costs.

5. Integration Algorithm

Centered space differences are used, together with an implicit 'alternating direction' method for time integration, yielding truncation errors of $\mathcal{O}(\Delta x^2, \Delta t^2)$ (Carnahan et al., 1969). This method is absolutely stable, but underestimates time trends in proportion to Δt . With $\Delta t = 15$ days inexpensive long integrations may be performed in which seasonal trends are adequately modeled. A shorter time step (e.g., 1 day) may be desirable for examining trends of a shorter time scale.

Negative mixing ratios are allowed but are rare and small and do not generally cause numerical instability.

6. Heterogeneous Removal Processes

Washout of HNO_3 and HCl is parameterized via specified altitude-dependent destruction rates in the troposphere.

7. Future Work

Ozone column amounts are somewhat sensitive to the details of how we specify the troposphere. We plan to carry out sensitivity studies and examine the lower boundary conditions carefully. We are also working with Dr. A.K. Smith of the University of Michigan to extend the domain to 120 km. Some thought needs to be given toward a representation of 'chemical eddies'. We will soon incorporate a vectorized detailed radiative code provided by Dr. J.T. Kiehl (another descendant of Ramanathan's code),

which should mitigate the cost of running the 'accurate' version. Finally, we are working on parameterizing the effects of Kelvin waves so that a self-consistent equatorial semiannual oscillation will occur in the model.

References

Ackerman, M., Mesospheric Models and Related Experiments, 149-159, 1972.

Brasseur, G., and P.C. Simon, J. Geophys. Res., **86**, 7343, 1981.

Carnahan et al., Numerical Methods, 1969.

Cunnold et al., J. Atmos. Sci., **32**, 170, 1975.

Garcia, R.R. and S. Solomon, J. Geophys. Res., **88**, 1379, 1983.

Hitchman, M.H., and C.B. Leovy, J. Atmos. Sci., in press, 1986.

Hitchman, M.H., and G. Brasseur, Rossby wave action as an interactive tracer in a 2-D model: parameterization of wave driving and eddy diffusivity, in preparation.

Holton, J.R., J. Atmos.Sci., **40**, 2497, 1982.

Kocharts, G., Planet Space Sci., **24**, 589, 1976.

Lindzen, R.S., J. Geophys. Res., **86**, 9707, 1981.

Nicolet, M., Geophys. Res. Letters, **6**, 866, 1979.

Nicolet, M. and W. Peetermans, Planet. Space Sci., **28**, 85, 1980.

Schoeberl, M.R., and D. F. Strobel, J. Atmos.Sci., **35**, 577, 1978.